

Pure spin decoherence in quantum dots.

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We uncover two microscopic physical settings with significant pure spin decoherence. First, for quantum dots (QD) electrostatically confined in two-dimensional hole gas, decoherence comes from qubit spin-orbit (SO) coupling to phonons, whose decay due to free charge carriers in contacts is described by Ohmic weighted phonon spectral function. We derive significant SO interactions affecting holes with origin and symmetry distinct from that of conventionally considered Dresselhaus and Rashba terms. In the second setting of electron or hole QDs coupled to a linear chain of atoms, decoherence is due to spin-dependent coupling to phonons, whose decay due to scattering off the free ends of a chain is described by the weighted phonon spectral function inverse proportional to frequency. The decoherence rate in both settings is linear in temperature.

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When spin population is conserved, quantum coherent properties are defined by pure spin decoherence[1]. In optics, there is a related phenomenon of zero phonon spectral lines[2–4]. For the field of quantum computing, understanding mechanisms of the pure spin decoherence is vital. In quantum dot (QD) qubits, the task is to uncover qubit-phonon interactions and processes in phonon system that lead to the effect. Current understanding of QDs does not include pure spin decoherence due to spin-orbit (SO) interactions and phonons as an effective mechanism, and finding to the contrary is important.

In this letter I show that pure spin decoherence is crucial for QDs. In particular, I consider QD qubits with charge carrier holes, in which spin relaxation is suppressed, and nuclear spin effects are weak compared to electron QDs. I derive spin-phonon interactions in hole QDs giving sizable pure spin decoherence. I show that steps can be taken to suppress it. I find that pure spin decoherence in QDs can be related to realistic microscopic mechanisms of phonon decay. It arises for a hole localized in a QD electrostatically confined in the two-dimensional (2D) gas, when the hole interacts with phonons, which in turn decay due to interaction with free holes present in the system, Fig.1. This is a microscopic realization of models with Ohmic phonon weighted spectral density. The other setting for pure decoherence, Fig.2, is electronic or hole QD coupled to 1D atomic chain, due to qubit-phonon coupling and phonon scattering of the free ends of the chain, which results in a weighted spectral density inverse proportional to frequency.

I derive the effective Hamiltonian for QDs confined to 2D hole systems, which also describes rings, wires and point contacts. The problem was extensively addressed in recent years [5–16], but an important effect was missed.

In the ground state of the confined hole systems, like heterostructures in iii-v or Si/Ge structures grown along 001 crystallographic direction, the effective mass m_h in the growth direction z is a heavy hole mass. This state is

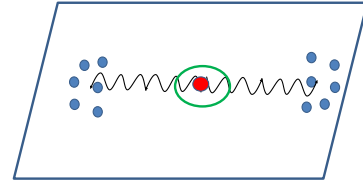


FIG. 1: QD in a 2D hole gas. Pure spin decoherence is due to interaction of a localized hole spin with phonons that in turn decay due to interaction with delocalized holes in contacts.

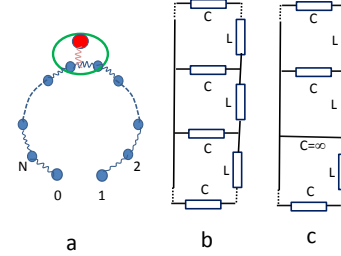


FIG. 2: a. QD coupled to a chain of atoms. Pure decoherence is due to spin coupling to phonons that scatter of the free ends (0,1) of a chain. b. Inductance-capacitance circuit equivalent to an ideal chain. c. Circuit for a chain with missing spring.

attractive for qubits [8], because it is mostly characterized by the angular momentum projection $L_z = \pm 3/2$. Since the matrix elements of spin-flipping interactions due to J_x and J_y between states $+3/2$ and $-3/2$ vanish, decoherence of hole QDs is reduced [17, 18] compared to electronic QDs. Understanding hole qubits requires knowledge of the effective Hamiltonian projected on the hole ground state doublet that must account for mixing of $\pm 3/2$ states to the states with light effective mass m_l in z -direction ($L_z = \pm 1/2$).

To date, SO interactions for 2D and QD holes have been treated similar to those for electrons, and limited to modified Dresselhaus and Rashba terms, which do not give pure spin decoherence. Here we show that SO interactions distinct from the Dresselhaus and Rashba terms affect 2D and QD holes. They arise even if bulk crystal is centrosymmetric (no Dresselhaus term [19]), and quantum wells (QW) are symmetric (no Rashba term [20]).

Their origin is the hole Luttinger Hamiltonian [21]

$$\mathcal{H} = \frac{1}{2m_0} \left((\gamma_1 + \frac{5}{2}\gamma_2)p^2 I - 2\gamma_2(\mathbf{J} \cdot \mathbf{p})^2 - 4(\gamma_3 - \gamma_2) \sum_{i>j} p_i p_j [J_i J_j] \right), \quad (1)$$

where J_i are the 4×4 matrices of the i -component of $J = 3/2$ operator, $[AB] = (AB + BA)/2$, γ_i are Luttinger constants, m_0 is the free electron mass. Infinite rectangular QW, in which Hamiltonian Eq.(1) is supplemented by the boundary conditions giving vanishing wavefunctions at $z = \pm d/2$, allows analytical solution [22–24]. Wavefunctions $\Psi_s(z)$, $\Psi_a(z)$ are symmetric and antisymmetric with respect to reflection about the plane $z = 0$, and in the basis of Bloch functions ($u^{3/2}, u^{1/2}, u^{-1/2}, u^{-3/2}$) describing bulk holes with $J = 3/2$, are given by $\Psi_{\pm}(z, \mathbf{r}) = a_{\pm}^{\mathbf{k}, z} \exp(i\mathbf{k} \cdot \mathbf{r})$, where \mathbf{r} is the in-plane coordinate, and

$$a_{-}^{\mathbf{k}, z} = \begin{pmatrix} iA_3 S_z e^{-3i\phi_k} \\ A_2 C_z e^{-2i\phi_k} \\ iA_1 S_z e^{-i\phi_k} \\ A_0 C_z \end{pmatrix}, \quad a_{+}^{\mathbf{k}, z} = \begin{pmatrix} A_0 C_z \\ -iA_1 S_z e^{i\phi_k} \\ A_2 C_z e^{2i\phi_k} \\ -iA_3 S_z e^{3i\phi_k} \end{pmatrix}, \quad (2)$$

\mathbf{k} is the in-plane momentum, ϕ_k is the angle between \mathbf{k} and x -direction. Here $S_z = \sin q_h z - (s_h/s_l) \sin q_l z$, $C_z = \cos q_h z - (c_h/c_l) \cos q_l z$, are antisymmetric and symmetric standing waves with respect to $z = 0$, $s_h = \sin q_h d/2$, $s_l = \sin q_l d/2$, $c_h = \cos q_h d/2$, $c_l = \cos q_l d/2$, and d is the QW width. For energies of in-plane motion $\epsilon_{\mathbf{k}} \ll \epsilon_q = \hbar^2 q_h^2 / 2m_h$, the wavevectors $q_h = \pi/d$ and $q_l = \sqrt{\nu} q_h$, where $\nu = m_l/m_h$. Thus, QW holes in contrast to QW electrons are described by two standing waves, illustrating mutual transformation of heavy and light holes upon reflection from the barrier. In the spherical approximation $\gamma_2 = \gamma_3$ and at small in-plane energies, the normalization factor $A_0 = \left(\frac{d}{2} + \frac{4\nu}{3} I_s \right)^{-1/2}$, $I_s = (1 + \frac{1}{s_l^2}) \frac{d}{2} + \frac{c_l}{s_l} \frac{(q_h^2 + 3q_l^2)}{q_l(q_l^2 - q_h^2)}$, and amplitudes $A_1 = A_0 \frac{\sqrt{3}k}{2q_h}$, $A_2 = A_0 \frac{\sqrt{3}k^2}{4q_h^2}$ and $A_3 = 3A_0 k^3 / (8\nu q_h^3)$.

Taking the projection [25] of $\hat{V}(\mathbf{r}, z, t)$ that includes potential confining holes to QDs and potential due to long-range hole-phonon interactions [26, 27] onto the ground state given by Eqs.(2), in the lowest order in \mathbf{k} we derive

$$\mathcal{H} = \frac{\hbar^2 k^2}{2m^*} + \alpha_0 \tilde{V}_0(\mathbf{r}, t) + \alpha_1 \tilde{V}_1(\mathbf{r}, t) - i\alpha_2 \mathbf{k} \cdot \nabla_{\mathbf{r}} \tilde{V}_1(\mathbf{r}, t) + \alpha_2 \sigma_z [\mathbf{k} \times \nabla_{\mathbf{r}} \tilde{V}_1(\mathbf{r}, t)]_z, \quad (3)$$

where m^* is the effective mass given by

$$\frac{m_0}{m^*} = \frac{\gamma_2(\gamma_1 + \gamma_2) - 3\gamma_3^2}{\gamma_2} + \frac{3\gamma_3^2(\gamma_1^2 - 4\gamma_2^2)^{1/2}}{\gamma_2^2} f(\theta), \quad (4)$$

where m_0 is the free electron mass, $f(\theta) = \frac{1 + \cos \theta}{\pi \sin \theta}$, $\theta = \pi \sqrt{\frac{\gamma_1 - 2\gamma_2}{\gamma_1 + 2\gamma_2}}$, $\alpha_0 = A_0^2 d$, $\alpha_1 = \frac{3A_0^2 k^2 d^3}{4\pi^2}$, $\alpha_2 = \frac{3A_0^2 d^3}{4\pi^2}$ and projection potentials $\tilde{V}_0(\mathbf{r}, t) = \frac{1}{d} \int_{-d/2}^{d/2} V((\mathbf{r}, z, t) C^2(z) dz$,

$\tilde{V}_1(\mathbf{r}, t) = \frac{1}{d} \int_{-d/2}^{d/2} V((\mathbf{r}, z, t) S^2(z) dz$. The SO terms in (3) give no spin-flips, and have $U(1)$ symmetry, partially breaking spin rotation symmetry [28]. Spin flip terms from projection of $\hat{V}(\mathbf{r}, z, t)$ onto $\Psi_{\pm}(z, \mathbf{r})$ contain at least the parameter $(kd)^3$ and are smaller than SO term in (3) at small in-plane energies. We note that for 2D holes, the Rashba term is $\propto k^3$, and the Dresselhaus terms include both cubic and linear in \mathbf{k} contributions [29]. Thus, the SO term in (3) missed in all previous work on hole QWs and QDs has profound consequences: in Si-Ge systems, it dominates; in iii-v systems, it changes the symmetry of SO interactions. This term is of sizable strength, defined by kd and averaging over z -direction, and is *not* related to admixture of distant bands like electron SO terms.

We now discuss pure decoherence in small QDs, with sizes less than hole mean free path. We take parabolic projection potential $\alpha_0 \tilde{V}_0 + \alpha_1 \tilde{V}_1 = m^*(\omega_1^2 x^2 + \omega_2^2 y^2)/2$ to model in-plane spatial confinement of holes. The linear in \mathbf{k} and \tilde{V}_1 term gives negligible mixture of orbital levels and is omitted. The relevant SO interaction is the last term in (3) due to hole-phonon interaction $V(z, \mathbf{r}, t)$. We will refer to it as spin-phonon interaction

$$\mathcal{H}_{sph} = \sigma_z \sum_{\mathbf{q}, j} V_{\mathbf{q}, j} (c_{\mathbf{q}, j}^{\dagger} - c_{-\mathbf{q}, j}) = \hbar \sigma_z \Omega_z, \quad (5)$$

where $V_{\mathbf{q}, j}$ is the Fourier component of the amplitude of spin-phonon interaction, j denote the phonon mode polarization, and $c_{\mathbf{q}, j}^{\dagger}$, $c_{\mathbf{q}, j}$ are phonon creation/annihilation operators, which define lattice displacement operator $\hat{\mathbf{R}}_{np} = \sum_{\mathbf{q}, j} \mathbf{u}_{np}(\mathbf{q}, j) (\hat{c}_{\mathbf{q}, j}^{\dagger} + \hat{c}_{-\mathbf{q}, j})$, where n labels the crystalline unit cell, p are the atoms in the cell, and

$$\mathbf{u}_{np}(\mathbf{q}, j) = \left(\frac{\hbar}{2\rho V \omega_{\mathbf{q}, j}} \right)^{1/2} \mathbf{d}_{\mathbf{q}, j} e^{i\mathbf{q} \cdot \mathbf{x}(np)}, \quad (6)$$

is the amplitude of the phonon in a mode \mathbf{q}, j at a site (np) , V is the crystal volume, $\mathbf{d}_{\mathbf{q}, j}$ is the phonon polarization vector, and $\mathbf{x}(np)$ is the lattice vector.

In calculating decoherence we assume the presence of uniform magnetic field $\mathbf{H} \parallel z$ with Larmor frequency ω_z . The projection of the spin operator σ_z is conserved. Hence, only pure decoherence can affect the qubit, once it is in a superposition of up and down state, with the pure decoherence constant Γ_{\perp} defining the motion of the transverse average spin:

$$\dot{S}_x = (\omega_z \times \mathbf{S})_x - \Gamma_{\perp} S_x. \quad (7)$$

For the spin-phonon interaction (5), $\Gamma_{\perp} = \Gamma_{xx} = \Gamma_{yy}$.

Our task is to find a microscopic mechanism(s), which result in non-zero Γ_{\perp} , and to calculate this constant. It is important to realize that spin-phonon interaction (5) will not lead to pure decoherence on its own. The effective magnetic field that acts on transverse spin due to this interaction is time and coordinate-dependent. If phonons are coherent and do not decay, they would result in coherent modulation of the ground and excited QD Zeeman

energy levels, with time-dependent phase. Indeed, at a given point in space, spin interaction with phonons is periodic in time. One frequent approach to decoherence is to introduce a phenomenological decay/correlation time. As we shall see, the overwhelming majority of phonon decay processes do not give Γ_{\perp} . In particular, although it was suggested [30] that spin-phonon interactions give decoherence because bulk phonons enter and leave the QD, such process cannot contribute on its own. The fact that spin-phonon interaction occurs only in a QD is accounted by the qubit wavefunctions defining $V_{\mathbf{q},j}$, and additional factors of phonon decay need to be considered.

To find out limitations on processes leading to pure decoherence, we calculate Γ_{\perp} , which is defined (see, e.g., [1]) by the Fourier component of the correlator of fluctuating spin-orbit fields at zero frequency

$$\Gamma_{\perp}(\omega = 0) = \frac{1}{2} \int_{-\infty}^{\infty} \langle \Omega_z(0) \Omega_z(\tau) \rangle d\tau, \quad (8)$$

where angular brackets denote statistical average. The correlator in Eq.(8) is defined by the Fourier image of the phonon correlation function $C(\omega) = \frac{1}{2} \sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 \langle c_{\mathbf{q}}^{\dagger}(\tau) c_{-\mathbf{q}}(0) \rangle + \text{h.c.}$, given by [31, 32]

$$C(\omega) = \frac{1}{\pi} \sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 \frac{(2N(\omega) + 1)\Pi(\omega)}{(\omega^2 - \omega_{\mathbf{q}})^2 / \omega_{\mathbf{q}}^2 + \Pi^2(\omega)}. \quad (9)$$

Here $N(\omega)$ is the number of phonons with energy $\hbar\omega$, and $\Pi(\omega)$ is the weighted phonon spectral function (in terms of Keldysh formalism, the imaginary part of retarded phonon self-energy). Real part of phonon self-energy, renormalizing phonon energy, does not result in decoherence and is neglected. We aim at finding $\Pi(\omega)$ on rigorous microscopic grounds, without introducing any phenomenological parameters of phonon decay.

The physics of dependence of Γ_{\perp} on $\Pi(\omega = 0)$ is that no energy exchange between Zeemann levels and phonons occur. SO hole-phonon interactions are only shaking up Zeeman levels. Physics is reminiscent of that of the zero-phonon line width in exciton or molecular absorption/emission [2–4]. However, spin dephasing and exciton linewidth problems differ. In the latter, carrier-phonon interactions give linear and quadratic in the phonon coordinates terms in two-level systems, and quadratic terms have been considered the principal cause of zero-phonon linewidth. In the former, the SO carrier-phonon term linear in phonon coordinates depends on σ_z , its square is spin-independent, and only the linear term can contribute to $\Gamma_{\perp}(\omega = 0)$. Some works [3, 4] conclude that interactions linear in $V_{\mathbf{q}}$ do not contribute to linewidth, or contribute only in the case of model localized phonons, rather than for realistic physical phonon/vibration modes. We now show two cases with real phonons contributing to relevant $\Gamma_{\perp}(\omega = 0)$.

In case I, $\Pi^I(\omega) = \omega/(2\omega_{\mathbf{q}}\tau_{\omega_{\mathbf{q}}}^I)$. Here $1/\tau_{\omega_{\mathbf{q}}}^I$ is the phonon decay rate at $\omega = \omega_{\mathbf{q}}$ for mechanisms giving

$1/\tau_{\omega}^I \propto \omega$. This is the case of Ohmic phonon spectral function, discussed in the theory of dissipative quantum tunneling by Leggett et al [33]. Here we calculate $\Gamma_{\perp}(\omega = 0)$ due to the process, in which phonons that interact with QD spin decay as a result of the phonon scattering off delocalized holes necessarily present in the system with electrostatically confined QDs. The case II, in which $C(\omega = 0)$ contributes to Γ_{\perp} , was never treated, and occurs when $\Pi^{\text{II}}(\omega) = \omega_{\mathbf{q}}/(2\omega\tau_{\omega_{\mathbf{q}}}^{\text{II}})$. Here $1/\tau_{\omega_{\mathbf{q}}}^{\text{II}}$ is phonon decay rate for mechanisms giving $1/\tau_{\omega}^I \propto 1/\omega$. We find the mechanism due to phonons interacting with qubit coupled to 1D linear chain, in which phonons decay due to scattering of the free ends, giving the case II.

By definition, $\Pi(\omega)$ is an odd function of ω . It is easy to see that cases I and II give the only possible dependencies of $\Pi(\omega)$ that contribute to non-zero meaningful $C(\omega = 0) = \lim_{\omega \rightarrow 0} C(\omega)$. The resulting $\Gamma_{\perp}(\omega = 0)$ is

$$\Gamma_{\perp}^I = \sum_{\mathbf{q}} \Omega_{\mathbf{q}}^2 \frac{k_B T}{\hbar \omega_{\mathbf{q}}^3 \tau_{\omega_{\mathbf{q}}}^I} \quad \text{case I}, \quad (10)$$

$$\Gamma_{\perp}^{\text{II}} = \sum_{\mathbf{q}} \Omega_{\mathbf{q}}^2 \frac{k_B T}{\hbar \omega_{\mathbf{q}}} \tau_{\omega_{\mathbf{q}}}^{\text{II}} \quad \text{case II}, \quad (11)$$

T is the temperature, k_B is the Boltzmann constant. Remarkably, $\Gamma_{\perp} \propto T$. This contrasts with known mechanisms of spin relaxation and decoherence in QDs, but is not surprising for pure dephasing, which, at $\omega = 0$, is similar to classical mean field fluctuations [34]. We note in passing that spin-independent QD electron-phonon interaction with consequent phonon decay due to electrons in contacts gives case I pure decoherence that can explain T^{-1} dependence of dephasing time in experiments [35].

We now turn to microscopic calculation of Γ_{\perp} .

Case I: In GaAs systems, the piezoelectric interaction of holes with acoustic phonons that defines the last term in Eq.(3) and spin-phonon interaction Eq. (5) is given by

$$\hat{V}(\mathbf{r}, t) = \sum_{\mathbf{q}, j} \beta_{ikj} e_k e_i \mathbf{d}_{\mathbf{q}, j} e^{i\mathbf{q} \cdot \mathbf{r} - i\omega_{\mathbf{q}, j} t} c_{\mathbf{q}, j}^{\dagger} \sqrt{\frac{\hbar}{2\rho V \omega_{\mathbf{q}, j}}} + \text{h.c.}, \quad (12)$$

where $\beta_{ikj} = \beta |\epsilon_{ikj}|$ is a piezoelectric constant, ϵ_{ikj} is an antisymmetric tensor, $\beta_{GaAs} = 1.2 \times 10^7 \text{ eV/cm}$, $e_i = q_i/q$. Denoting $\lambda_i = \sqrt{\hbar/m^* \omega_i}$ the sizes of the wavefunctions ϕ in 1D parabolic potentials, we find the QD orbital ground state wavefunction $\Psi \simeq \Psi_{00} + b\Psi_{11}$, where $\Psi_{nm} = \phi_n(x)\phi_m(y)$, and $a = i\omega_c(\lambda_1/\lambda_2 - \lambda_2/\lambda_1)/4(\omega_1 + \omega_2)$. In weak magnetic field, the lowest QD states are due to Zeeman doublet of the ground orbital state.

The hole-phonon interaction \tilde{V}_2 in Eq.(3) defined by (12) gives $\Omega_z \propto \langle \Psi^* | e^{i\mathbf{q} \cdot \mathbf{r}} (q_x k_y - k_x q_y) | \Psi \rangle = a(q_x^2 \lambda_x / \lambda_y - q_y^2 \lambda_y / \lambda_x)$. It also leads to factor $A(\mathbf{q}) = \sum_j |\mathbf{d}_{\mathbf{q}, j}|^2$ entering $|V_{\mathbf{q}}|^2$ in Eq. (9). In a simple model with isotropic speed of sound s , $A(\mathbf{q}) = (q_x^2 q_y^2 + q_y^2 q_z^2 + q_z^2 q_x^2)/q^4$.

Calculating $\Pi(\omega)$ due to interactions of phonons with holes in contacts, we neglect renormalization of the hole-phonon vertex, like in consideration [31] of electron-

phonon interactions in 3D metals. In the 2D case

$$\Pi_{\mathbf{q}}^I(\omega) = \frac{\hbar\beta^2 A(\mathbf{q})}{2\rho\omega_q d} \int G(\mathbf{p}, \epsilon) G(\mathbf{p} - \mathbf{q}, \epsilon - \omega) d^2 p d\epsilon \quad (13)$$

where $G(\mathbf{p}, \epsilon)$, ϵ_F and p_F are the Green function, Fermi energy and momentum for holes in contacts. At small ω

$$\Pi_{\mathbf{q}}^I(\omega) = \frac{\beta^2 m_* A(\mathbf{q})}{4\pi\hbar d \rho \omega_q} \frac{p_F}{q} \frac{\hbar\omega}{\epsilon_F} \Theta(2p_F - q), \quad (14)$$

where $\Theta(x) = 1$ at $x > 0$ and $\Theta(x) = 0$ at $x < 0$.

Calculating the hole ground state diagonal matrix element of (12), evaluating Eq.(14), and taking $\omega \rightarrow 0$ in Eq.(9), for $m_* = 0.25m_0$, hole density in contacts $p = 6 \times 10^{11} \text{ cm}^{-2}$, $s = 4 \times 10^5 \text{ cm/s}$, $d = 100\text{\AA}$, $\lambda_x = 400\text{\AA}$, $\lambda_y = 250\text{\AA}$, $H = 0.5T$ and $T = 100\text{mK}$, from Eq.(10) we get $\Gamma_{\perp}(\omega = 0) = 10^4 \text{ Hz}$. Thus, pure decoherence is significant in GaAs QD. This rate exceeds 10 times the hole decoherence rate experimentally observed in InAs QD [36]. To fight the pure decoherence, one makes QD shape close to circular. We note that in SiGe/Ge/SiGe QD structure, our estimates show $\Gamma_{\perp}(\omega = 0) = 10^3 \text{ Hz}$ for similar QD sizes. With decoherence due to nuclei in such structures weaker than in GaAs, pure dephasing proposed here becomes important. We address hole qubits in Si/Ge structures elsewhere[18].

Phonon decay due to anharmonic processes, scattering by impurities, surfaces, or QD or QW boundaries gives $\Pi(\omega) \propto \omega^s$ with $s \geq 3$ and does not lead to case I pure dephasing. Therefore observation of pure dephasing will make it possible to separate phonon decay due to charge carriers in contacts from all other decay mechanisms.

Case II: This setting can be realized in QD coupled to 1D linear atomic chain, where phonon decay occurs due to scattering off its free ends. Spin-phonon term (5) can arise in both electron and hole QDs due to g-factor fluctuations [37]. For case II in electron QDs, we consider g-factor modulation in a QD of wavefunction extent λ by phonons of a chain of N atoms of mass M with lattice constant a linked by nearest neighbor springs of spring constant η . Following [38], we get interaction (5) $V_q = i(\hbar/2MN\omega_q)^{1/2} A q e^{-q^2 d^2/4} \hbar\omega_Z$, where $\omega_q^2 = (4\eta/M)\sin^2(qa/2)$, and A is a constant, which can be obtained from spin resonance experiments [39]. We consider ends as defects in crystal with cyclic boundary conditions. In this model, $\Pi_q^{II}(\omega) = \frac{2\pi}{\hbar} \sum_{\mathbf{q}'} |\langle \mathbf{u}_{\mathbf{q}'} | T(\omega + i0) | \mathbf{u}_{\mathbf{q}} \rangle|^2 \delta(\hbar\omega - \hbar\omega_{\mathbf{q}'})$. Here $\mathbf{u}_{\mathbf{q}}$ is given by Eq.6 in 1D case, scattering matrix $T(\omega)$ with dimensionality of a spring constant is defined by Dyson equation $T = \delta L + \delta LGT$, G is the ideal chain phonon Green function, δL is perturbation in spring constants due to chain ends at atoms $n = 1$ and $n = 0$, with zero γ of spring joining them. The nonzero $\delta L_{nn'}$ are $\delta L_{00} = \delta L_{11} = -\delta L_{10} = -\delta L_{01} = \eta$. Expanding $T(\omega)$ in $\mathbf{u}_{\mathbf{q}}$ as $T_{nn'}(\omega) = 2M^2/\hbar \sum_{q_1, q_2} u_n(q_1) t(q_1, q_2, \omega) u_{n'}(q_2)$,

from the solution of Dyson equation[40] we find

$$t(q_1, q_2, \omega^2 + i0) = \frac{4\eta e^{-ia(q_1+q_2)/2} \sin \frac{q_1 a}{2} \sin \frac{q_2 a}{2}}{M\omega^2 \sum_q [\omega^2 - \omega_q^2 + i0]^{-1}}. \quad (15)$$

Eq.(15) gives $t \propto 1/\omega$ that is key to singular weighted phonon spectral function and Γ_{\perp}^{II} :

$$\Pi_q^{II}(\omega) = 2\eta |\sin qa/2|/M\omega \quad (16)$$

$$\Gamma_{\perp}^{II} = 4(\omega_Z/\omega_L)^2 \cdot (kT/\hbar\omega_L) \cdot (A^2 \hbar/M\lambda a), \quad (17)$$

where $\omega_L^2 = 4\eta/M$. Physics of $t \propto 1/\omega$ resulting in such Π_q^{II} is clear from the electrical circuit equivalent to an atomic chain with missing spring, Fig 2c. At capacitance $C = \infty$ (due to $\gamma = 0$ between ends 0 and 1), the circuit is shorted, and $\omega \rightarrow 0$ response to finite current J is zero voltage V (the response to finite V is $J \propto 1/\omega$). In a chain with free ends, finite force gives displacement $\propto 1/\omega$; when phonons scatter, $t \propto 1/\omega$. Taking $\lambda = 50\text{\AA}$ for a carbon QD coupled to a chain of carbon atoms with $M = 2 \times 10^{-23}\text{g}$, $a = 2.5\text{\AA}$, $\omega_L = 1.2 \times 10^{11} \text{ Hz}$, $A = 0.1$, $H = 0.5T$, $T = 100 \text{ mK}$, we get $\Gamma_{\perp}^{II} = 10^7 \text{ Hz}$. Such decoherence must be avoided. This shows, e.g., the limits on reducing bath dimensions in engineering qubits. Once phonons are 3D, case II is not realized. We note here that decay rates Γ_{\perp}^I and Γ_{\perp}^{II} are not additive: once case II decoherence is present, Γ_{\perp}^{II} solely defines Γ_{\perp} .

In conclusion, we demonstrated that pure dephasing can considerably affect qubits in important settings. We presented two physical mechanisms based entirely on realistic microscopic quantum processes, without introduction of any kind of phenomenological correlation time. We also demonstrated that important spin-orbit interactions distinct in origin and symmetry from known Rashba and Dresselhaus terms describe physics of low-dimensional holes. Support by NSF grant ECCS-0901754 is gratefully acknowledged.

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